Research Matters

annual report 2014-2015

ACENET
accelerate discovery

computecanada
regional partner

Contents

Celebrating 12 Years of Success

Today, computers are everywhere. They assist us in the home with mundane tasks, in the workplace with our efficiency, and in our moments of leisure with entertainment.

But that's not all they can do. Advanced computing has the power to shape the future! With the right expertise, resources and vision, advanced computing can help find solutions to some of the world's greatest problems. In the past year alone, extraordinarily innovative research initiatives have benefited from ACENET's advanced computing resources in all four Atlantic provinces.

ACENET is home to one of Canada's most advanced computing networks. Its human capital is unique. ACENET's experience in applying advanced computing to difficult research problems is equal to the best. ACENET is also recognized as one of the best managed advanced computing networks in Canada. Over the twelve years of its existence, ACENET has grown, expanded its services, improved the quality of its delivery, and supported Atlantic Canada's research community in achieving world-class research outcomes. ACENET is living proof of the power of partnership in Atlantic Canada. I invite you to learn more about us by reading this report.

Most Sincerely,

Dr. Richard J. Marceau, PEng, PhD, FCAE
Chair, ACENET Board

The Path Ahead

I am very pleased to present our first annual report. It has been an exciting year for ACENET with many changes and enhancements which will set the stage for our continued evolution in the coming years.

On the Compute Canada front, 2014 saw the addition of a new CEO (Mark Dietrich) and CTO (Greg Newby) which facilitates a much needed higher level of cooperation and coordination between the regional consortia. A critical CFI funding condition was achieved in 2014 through selection of the four core hosting locations for Compute Canada. ACENET and its member institutions fully support this decision and will continue to participate in the delivery framework used to operate and maintain these centres.

The road ahead is an exciting one for ACENET. Our team is fully engaged and the events of 2014 have inspired us to once again refocus our efforts, architecting a new future and building on our core strengths and expertise. We look forward to a continued partnership with Compute Canada and to an evolving and exciting next year and beyond, and now more than ever, we remain fervently committed to our research family here in Atlantic Canada and to delivering value at every step of the way.

Sincerely,

Ray Miller, P.Eng.
Executive Director, ACENET

Accelerating Discovery with ACENET

Accelerating discovery and innovation is the driving force behind ACENET. With a dedicated team of experts throughout the region, we provide advanced computing resources and expertise to researchers and industry throughout Atlantic Canada. Through our activities, we accelerate discovery and innovation, help attract and retain highly qualified people in the region and empower students with foundational skills in the high-demand field of advanced computing.

Initially founded to serve computationally-based research needs at five universities across Atlantic Canada, ACENET's membership has since grown to nine universities and nearly 900 users. During the past 12 years, we've become an indispensable resource, serving not only researchers at any institution in the region, but government departments and qualifying private companies as well. We are a regional partner with Compute Canada, the national organization responsible for advanced research computing in Canada. Through this partnership, we provide access to resources from across the country and represent our regional interests at the national table.

Highlights From 2014-15

Excellence in Research

Each year, Compute Canada awards additional computing resource allocations through a national competition. This year, a number of researchers in Atlantic Canada were awarded additional allocations in recognition of their research excellence:

- Dr. Richard Karsten, Acadia University, Tidal Energy
- Dr. Randall Martin, Dalhousie University, Air Quality and Climate
- Dr. Chris Beaumont, Dalhousie University, Geodynamics
- Dr. Katja Fennel, Dalhousie University, Marine Environmental Modeling
- Dr. Julie LaRoche, Dalhousie University, Marine Biology
- Dr. Erika Merschrod, Memorial University, Optical Response of Sensor Films
- Dr. Jahrul Alam, Memorial University, Atmospheric Turbulence
- Dr. Travis Fridgen, Memorial University, Impact of Specific Ions on DNA
- Dr. Valerie Booth, Memorial University, Lung Surfactant
- Dr. Christopher Rowley, Memorial University, Computational Methods for Biophysical Chemistry
- Dr. Paris Georghiou, Memorial University, Organic Chemistry
- Dr. Entcho Demirov, Memorial University, Ocean Modeling & Data Assimilation
- Dr. Hossain Farid, Nova Scotia Agricultural College, Animal Breeding & Genetics
- Dr. Kai Ylijoki, Saint Mary's University, Oil Sands Upgrading

ACENET also supports 12 Canada Research Chairs.

Industry Affiliations

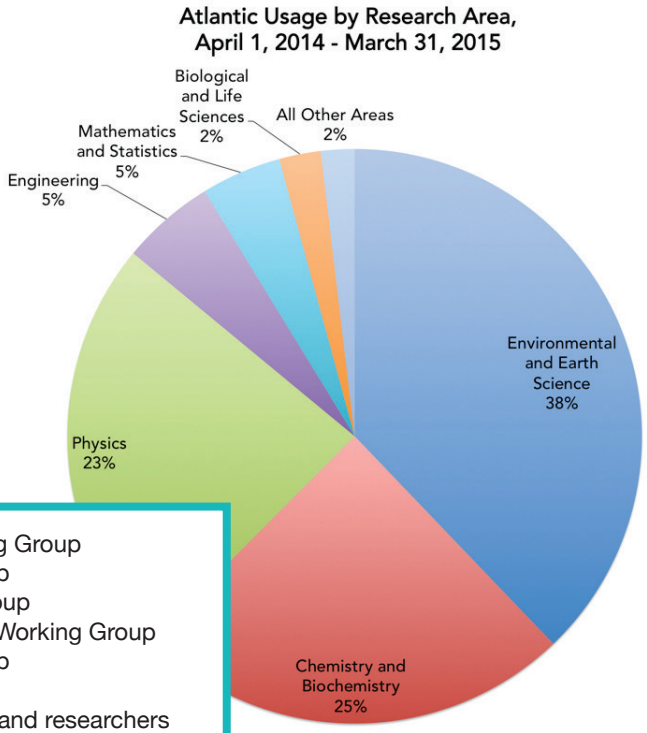
As part of our commitment to regional economic development, ACENET began forging relationships directly with industry and with agencies that support start-ups and the commercialization of research. Many of our researchers already partner with industry.

Training

Providing skills training in advanced research computing to students and researchers is a key component of ACENET's mandate. In addition to the many one-on-one and small group sessions, our Computational Research Consultants carried out 28 formal training events in 2014-15. ACENET is pleased to be supporting over 500 students in research projects.

2014 High Performance Computing Symposium

In June of 2014, ACENET hosted the annual national High Performance Computing Symposium, Canada's premier supercomputing event. Boasting one of the highest participation rates on record, 275 researchers, technicians, and representatives from industry and government attended the main conference, with 50 participating in the technical tutorial sessions. Partnering with NSERC, Springboard Atlantic and Dalhousie University, we also hosted a pre-symposium connector event entitled Academic-Industry Dialogue on Big Data Analytics. This panel discussion packed the room with 85 representatives from business, government and other parts of the advanced research computing sector.



ACENET Research Fellowships

Another round of ACENET Research Fellowships was launched in the fall of 2014. A total of $250,000 of the $440,000 two-year allocation has been committed to date. We are thrilled to be supporting 13 graduate and 24 undergraduate students throughout the region in their research.

Contributions to the National Scene

ACENET's technical staff takes on many special projects such as building portals, developing backend tools, managing equipment for dedicated computing resources and supporting regional projects. As one of the four regional partners that make up Compute Canada, ACENET's small but impassioned staff of 15 play a significant role on the committees and working groups that make Compute Canada tick. Some of the national groups our people participate in include:

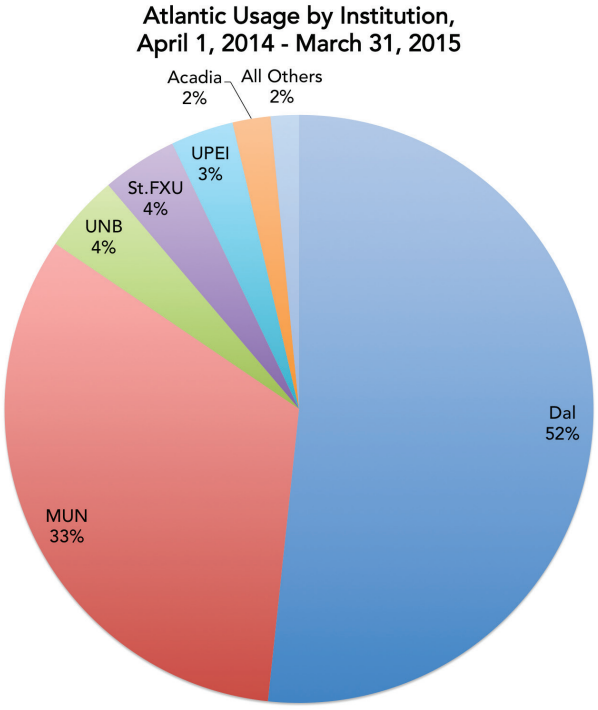
National Executive Committee
Council of CTOs
National Communications Committee
National Resource Allocation Committee
Finance & Administration Committee

Site Selection Internal Review
National Security Council

Education/Outreach/Training Committee
Research Support Committee
National Platform Committee
Physical Infrastructure Committee

Cloud Working Group
Biosimulation Working Group
Access to Resources Working Group
Digital Humanities Working Group
Accelerator Working Group
Collaboration Working Group
National Support System Working Group
Networking Working Group

Our Research Directorate and researchers also supported a number of Compute Canada's regional consultations and town halls during the year, addressing subjects such as Compute Canada's national strategy, cyber-infrastructure planning, and the reduction of datacenter sites. Atlantic Canada was well represented at these sessions.



Developing Tidal Energy

In Dr. Richard Karsten's office at Acadia University the entire Bay of Fundy has been reduced to a grid made up of 100,000 triangles displayed on an oversized computer screen. The data points – tide height, current and water depth – have been carefully plotted by the mathematics professor and his graduate students to create a computer model that can pinpoint the nature of the tide at any spot on the bay at any given second for the next 25 years. It's a staggering amount of data.

"At the basic level, what we're studying is how fast the water is flowing at any given point," he says. "Then we get into more detail and look at things like the variations in the direction and speed of flow."

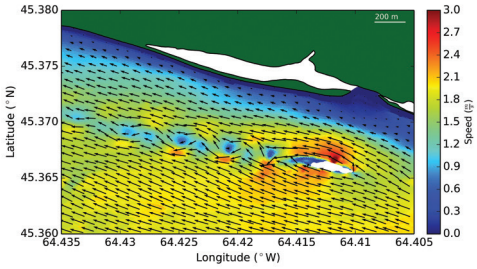
The 270 kilometre-long bay Karsten is studying is one of the most unique places on Earth; a submerged rift valley where the world's highest tides rise over 16 meters daily, moving 160 billion tonnes of seawater in the process, and powering a dynamic ecosystem teaming with life. It's a place often mentioned in the same breath as the Great Barrier Reef and the Amazon. A place where a dozen species of whales regularly congregate and millions of shore birds gather every year to fatten themselves up for their migration to South America. Not only is it visually spectacular, it could also be North America's next great source of hydroelectric power.

A number of projects are underway to harness those powerful tides. Most notable is the Fundy Ocean Research Centre for Energy or FORCE, a government and industry supported test centre for in-stream tidal energy located in Parrsboro, Nova Scotia. There are smaller projects as well, including one by Fundy Tidal Inc., a corporation headquartered on Brier Island Nova Scotia. Fundy Tidal is partnering with Clean Current Power Systems Inc. of British Columbia to develop five small community tidal projects to sell energy through Nova Scotia's Community Feed-In Tariff (COMFIT) program.

Karsten's research, along with information provided by project partners Dalhousie University, the University of New Brunswick and Dynamic Systems Analysis, will provide information for those projects by locating the spots where engineers can best place underwater turbines, along with long term projections of just how profitable those turbines will be. "Numerical models are relatively cheap as opposed to testing," he says. It is one reason his research has attracted funding support from Natural Resources Canada, the Offshore Energy and Research Association of Nova Scotia and NSERC.

Karsten's research provides critical support to the development of a tidal energy industry both in Nova Scotia and nationally. Such an industry would produce substantial amounts of sustainable, renewable electricity that would reduce Nova Scotia production of greenhouse gases and decrease its dependency on foreign fuels. Last year, some of his research activities included making extractable power estimates for all major Nova Scotia tidal resources. In total, the calculations estimated that the tidal resource could support over 1400 MW of installed capacity with only a minor impact on the tides. This is 55% of Nova Scotia generation capacity.

Karsten has six students in his research group and has received additional computing resources for 2015 through Compute Canada's national Resource Allocation Competition.



The tidal flow past Black Rock in Minas Passage, as simulated using the Acadia-FORCE Numerical Model. The strong tidal flow past Black Rock produces a kilometre-long, undulating wake. The location and dynamics of the wake are important in deciding the deployment location of tidal turbines.

Why Materials Do the Things They Do

Dr. Geoffrey Lee-Dadswell is a theoretical physicist at Cape Breton University, who for the past 15 years has been studying why materials do the things they do. Specifically, he studies heat and momentum transport on a very small scale.

For an example of large scale heat transport, take a frying pan on a stove. We know that the stove element heats the bottom of a pan to the point that food cooks. However, the handle of the pan doesn't get as hot. Why? The answer lies in understanding the transport of heat, which obeys Fourier's Law of Heat Conduction. This law has been known for almost 200 years, but surprisingly, is not well understood.

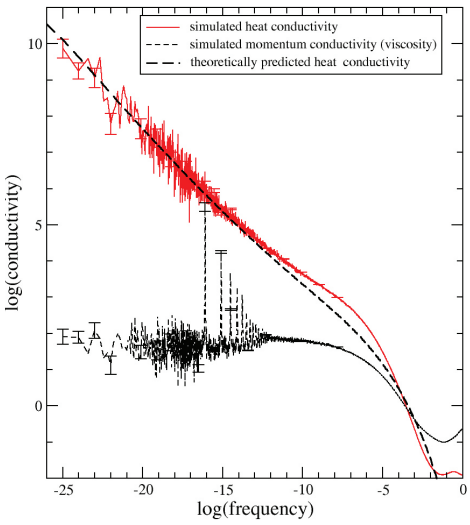
One of the mysteries about Fourier's Law is that it doesn't seem to work for some objects on the nanometre-scale. A nanometre is one billionth of a metre. If you were to lay atoms across a nanometre, you might fit only about 10! Computers for example have become faster largely because the parts of their chips have been made smaller over the years. As this process continues, more and more parts of an ordinary desktop computer or smart phone are nano-electronics.

Lee-Dadswell studies nano-systems that are one-dimensional, which is to say that for theoretical purposes, they have only length. Now because we live in a three-dimensional world, everything has a width and a depth. However, in some nano-systems, these are so small that they can be ignored. Examples of one-dimensional systems are polymer chains such as the polyethylene chains that pop bottles are made of and carbon nano-tubes (think of these like a sheet of graphite that's been rolled up into a tube). Carbon nano-tubes are often a few micrometres long, but can be only five to ten nanometres wide.

Physicists once believed that everything obeyed Fourier's Law of Heat Conduction, but researchers have found that these one-dimensional systems behave differently from other systems – disobeying Fourier's Law. Moreover, they don't know why, which also means that they don't have a solid understanding of why everything else does obey Fourier's Law. Physical laws are preferably derived from the more fundamental mechanics, but nobody knows how to derive Fourier's Law from mechanics. If they can't derive it, then they really don't understand the law. This drives physicists nuts! It means that we don't understand things like heat flow as well as we thought. This puzzle began to surface in the early 1900s, but didn't come to the forefront until the 1970s. It's challenging to make progress on such a long-standing mystery, and tackling it is therefore rather scary. Lee-Dadswell is one of only a few researchers in the world doing so.

Lee-Dadswell generally has one or two undergraduate students working with him. He develops models, and the students then run dozens of simulations in parallel on ACENET systems, each running for possibly weeks and involving tens or hundreds of thousands of atoms interacting with each other.

By understanding the fundamental laws of transport, solving problems such as removing heat from nano-electronics and improving refrigeration technology become possible.



The curves in the graph show the heat conductivity and viscosity of a one-dimensional system as a function of the frequency of vibrations in the system that are carrying the heat or momentum. The viscosity curve "flatlines" at low frequency. This is the conventionally expected behaviour, but turns out to be unusual in one-dimensional systems. The heat conductivity gets bigger and bigger as we look at lower frequencies. This is not what Fourier's Law predicts, but turns out to be what we usually see in one-dimensional systems. The theoretical curve, which follows the simulation very well at low frequencies, is generated by Lee-Dadswell's theory.

Tracking Air Pollution

The health hazards and environmental impacts of emissions from industry, vehicles and other sources are well established: cardiovascular disease, asthma and premature deaths, as well as crop damage and disease outbreaks in certain tree species. Yet little is known about how particulate matter – tiny invisible specks of mineral dust, carbon and other chemicals – moves through the atmosphere and its effects on the health of local populations around the world.

That's changing thanks to the work of Dr. Randall Martin, an atmospheric scientist who uses remote sensing satellites, computer modeling and advanced research computing to identify the trends and magnitude of human exposure to these pollutants. These tools allow his group to collaborate with Health Canada and Environment Canada to contribute to science-based decision making to protect the health and well being of Canadians.

The Atmospheric Composition Analysis Group at Dalhousie is the only research group in the world that has applied satellite remote sensing to infer long-term concentrations of global, ground-level fine particulate matter. Traditional ground-based instruments for monitoring air pollution are located primarily in urban areas, leaving rural and remote communities with no data on the quality of the air they breathe. Martin's group is able to paint a more comprehensive and accurate picture of air pollution for geographic regions as small as 10 kilometres, using publicly available satellite data generated over the past decade from space agencies around the world, including NASA.

"NASA has invested billions of dollars in the preparation and launch of these satellites and in the data collection, and for relatively modest investments here in terms of computing and people, his group can leverage that substantial investment," says Martin.

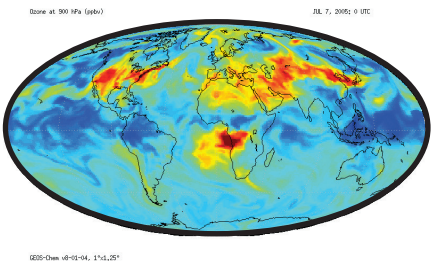
The biggest surprises from the research have been in areas of south and east Asia, north Africa and the Middle East where coal-fired generating plants and wind-blown mineral dust have contributed to significant air pollution. Other pollution "hot spots" were identified over eastern North America and northern Europe.

This research is helping scientists and policymakers understand how chemicals in the atmosphere affect climate change and air quality. The Canadian government used Martin's data to develop more stringent and comprehensive air quality standards for fine particulate matter, a major component of smog. His team's work has also contributed to several high-profile global assessments conducted by the Organization for Economic Co-operation and Development (OECD), the World Health Organization (WHO) and other international agencies.

Martin's group has also had a leading role in the development of an open-source, global, three-dimensional model of atmospheric composition called GEOS–Chem, which is used by more than 70 institutions worldwide. It allows assessment of sources and processes that affect air quality.

"One possible benefit from our research is increased life expectancy for people around the world due to improved policies that clean the air that we breathe," says Martin. "It could also contribute to a better understanding of the effects of human activities on climate change and lead to more informed decisions about how we might best deal with this complex issue."

Dr. Martin typically works with 15 to 20 students and postdocs, and has received additional computing resources for 2015 through Compute Canada's national Resource Allocation Competition.



Developing Artificial Lung Surfactant

Lung surfactant is a material that lines the air-sacs in the lungs and is essential for breathing. Premature babies are often born before they have a chance to produce sufficient lung surfactant and they need to be given it in order to help them breathe. This surfactant is generally sourced from animals.

People of any age who are seriously ill or injured also frequently have damage to their lung surfactant, which impairs their ability to breathe. One such condition, called Acute Respiratory Distress Syndrome (ARDS), affects 150,000 people per year in the US, and has a fatality rate of about 40%. Unlike with premature babies, treating adults with surfactant derived from animals has been very challenging for two reasons. First, adult lungs are larger than a baby's and it's therefore difficult to get enough animal surfactant together to cover it. Second, there are hostile conditions present in the lungs of ARDS patients that deactivated their own lung surfactant, and that rapidly inhibits surfactant.

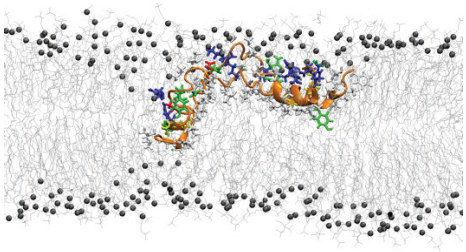
Dr. Valerie Booth is working with a multi-disciplinary team at Memorial University and a research team in Spain to understand the essential features of the proteins in natural lung surfactant and to use this knowledge to develop artificial lung surfactant treatments that are more resistant to deactivation.

Specifically, Booth's research focuses on Surfactant Protein B (SP-B). SP-B is of particular importance because unlike the other lung surfactant proteins, you absolutely can't live without it in your lungs. Furthermore, unlike most essential proteins, we strangely do not know the three-dimensional structure of SP-B, or what it looks like. Consequently, we don't understand how it works. This is because SP-B is exceptionally hard to work with experimentally.

SP-B is very hydrophobic, a fancy word for sticky. It likes to stick to greasy, lipid molecules instead of to water. Despite the challenges, it is possible to use experimental techniques to find out small pieces of information about its structure. However, the key to unlocking SP-B's molecular structure is through running simulations on Compute Canada infrastructure. Booth's group uses these simulations to make predictions about what SP-B looks like, and then compares those to the experimental data in order to provide the best possible picture of SP-B.

Proteins are like tiny molecular machines and we can't figure out how they work until we know what they look like. Determining what SP-B looks like tells researchers how it works. Understanding how we breathe will help Booth develop a treatment for ARDS. In fact, she, two of her PhD students and a research assistant are currently working towards a provisional patent for a formulation for artificial surfactant, with the hope it will result in an industrial partnership.

Dr. Booth has received additional computing resources for 2015 through Compute Canada's national Resource Allocation Competition.



Simulation of SP-B's structure within surfactant lipids.

Oil Sands Upgrading Methodologies

The Alberta oil sands are the world's third largest proven source of oil in the world and comprise 140,200 square kilometres. The majority of oil extracted there involves pumping high bitumin concentrated underground deposits to the surface, where the bitumin is then extracted from other components. Once this is done, it is upgraded to Synthetic Crude Oil, which is then refined for products we use daily.

However, the extraction process is dirty, containing harmful chemicals such as sulphur and nitrogen. Upgrading and refining the oil for fuel and heat consumption means removing those dirty components. At the moment, the process of upgrading oil from Alberta's oil sands is neither as efficient, nor as environmentally friendly as it should be. This has led to domestic and international criticism.

For the past year and a half, Dr. Kai Ylijoki at Saint Mary's University has been working with a team at the Institute for Oil Sands Innovation (IOSI) at the University of Alberta. IOSI's vision is to have "Oil sands operations with a reduced environmental footprint by minimizing water use, consuming less energy, lowering greenhouse gas and other emissions, yielding high quality products at lower cost." [http://www.iosi.ualberta.ca]

Key to achieving this vision is understanding the complexes in the oil – what they are, their molecular structure, and the mechanism by which they work in upgrading.

Dr. Ylijoki is, among other things, a computational chemist and his work involves studying these complexes with a view to identifying better catalysts. He does this by studying their properties to better understand their behaviour. The large size of the molecules renders them impossible to study on standard desktop computers, so he uses ACENET and Compute Canada's advanced computing resources.

Once he understands the complexes, then it's a matter of finding very active catalysts for bond activation that don't require large quantities, do the job more efficiently and are more environmentally friendly. IOSI has had success in this area – breaking certain complexes selectively – and finding ways to quicken the catalyst. Through the computational work of Dr. Ylijoki and his two students, the IOSI team is excited to be seeing some other unique aspects to the complexes that could be applied to other industries.

Finding more efficient, environmentally better ways of cleaning oil from Alberta's oil sands will help Canada economically, environmentally, and internationally.

Dr. Ylijoki has received additional computing resources for 2015 through Compute Canada's national Resource Allocation Competition.

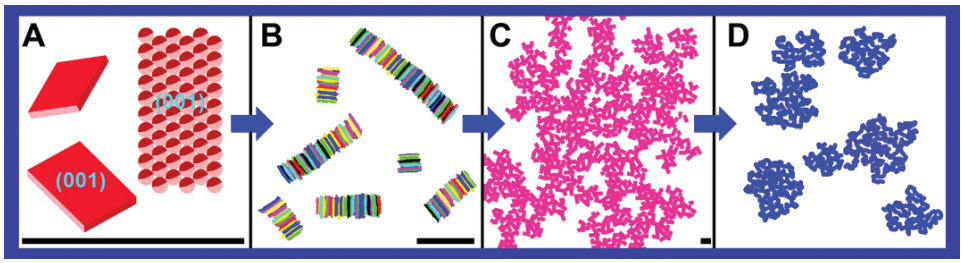
Edible Oils

Have you ever wondered why foods contain trans fats, or why dough needs so much salt, or why cheese tastes so good?

Dr. David Pink at St. Francis Xavier University is a theoretical physicist working on edible oils, with the intent of making them healthier for people to eat. Food companies will have to replace certain trans fats in their products and the big question is "by what can they be replaced?" The problem arises from the fact that (solid) trans fats help create liquid oil-binding structures in products such as shortenings. Without their "Oil Binding Capacity", shortenings and similar products just won't work. But, industrially-manufactured trans fats created via hydrogenation have been shown to damage human health and the US Food & Drug Administration (USFDA) will require producers to cease using them. Accordingly, to replace them, we need alternatives that are inexpensive, edible and behave the same way as trans fats so that consumers won't be able to tell the difference.

Working in collaboration with Dr. Alejandro Marangoni, Professor of Food Science at the University of Guelph, the process begins with trying to understand what solid fats structures arise in edible oils and why they trap the oil so as to exhibit the desired Oil Binding Capacity. Without understanding those fundamental things, researchers can only make, at best, educated guesses as to what ingredient can be used to successfully replace them – an inefficient way to try to solve a multimillion dollar problem.

Instead, Pink began by modelling crystalline nanoplatelets, the most stable small solid fats in the oils, then simulated their interactions to study them. Because of the models' complexity - edible oils involve many components - he had to make use of computer simulations, working with his Research Associate, Bonnie Quinn, and using ACENET. The goal was to predict what structures develop in edible oils. Pink says, "If it wasn't for ACENET, I wouldn't even be able to begin.".



The predicted Hierarchy of Aggregation in some edible oils.
A: Crystalline nanoplatelets. B: TAGwoods. C: TAGwood aggregation Into a DLCA/RLCA cluster. D: Uniformly distributed DLCA/RLCA clusters. The horizontal black bar shows a scale of ~500-1000 nm. DLCA: Diffusion Limited Cluster Aggregation; RLCA: Reaction Limited Cluster Aggregation.

Pink predicted the experimental structures which arise in systems using ultra-small angle X-ray scattering (USAXS). He also predicted the existence of stacks of crystalline nanoplatelets, called TAGwoods. His predictions were all confirmed by his PhD student. He then made predictions about solid fats which become coated with semi-liquid oil components. He, Dr. Shajahan Razul of ACENET and Pink's undergraduate student carried out atomic scale molecular dynamics simulations and showed that Pink's assumptions about coated solid fats were justified and that they will indeed bind oil. Subsequent projects will address how larger structures get formed, so that he can begin searching for replacements for trans fats.
One such project will probe the dynamics of edible oils using dissipative particle dynamics, a simulation technique that can study larger scale systems over longer timescales.

In recent months, Pink has branched out. With Dr. Marangoni's leadership and an industry collaboration, he is modelling cheeses to discover the essential aspects of their structures.

Pink is also modelling dough. Bread makers will be required to reduce the amount of salt and this can make the dough sticky. Working with Dr. Erzsebet Papp-Szabo, who provides input about the chemistry of dough, he has just finished developing models and has some preliminary results.

Now in his 70s, by most people's standards, David Pink should be retired. "But," he said, "I'm simply having too much fun working with Alejandro, with my other colleagues and with my students." And he is pleased that his work has been recognized by the 2015 Distinguished Service/Outstanding Achievement Award from the Edible Applications Technology division of the American Oil Chemists' Society.

New Tools For Designing Safer Chemical Catalysts

Dr. Ghislain Deslongchamps leads a small group of researchers at the University of New Brunswick, adapting computational chemistry tools normally used in drug design for discovering new catalysts with a wide range of applications – and not just any kind of catalyst.

A catalyst is a small molecule that accelerates a particular chemical reaction. One type of extremely valuable catalyst is one that promotes a chemical reaction to generate a molecule as a single stereoisomer. Stereoisomers are molecules that are identical except that they mirror each other's structure. The analogy used by Deslongchamps is a pair of gloves. The two gloves are exactly the same except that the left glove is a mirror image of the right; each glove can only fit its respective hand. The same applies to drug molecules and how they interact with the body, so they typically need to be produced in the correct 'handedness' in order to be safe and effective. For example, thalidomide was a drug sold in the late 1950's to treat morning sickness in pregnant women. It was manufactured as a 50:50 mixture of its two stereoisomers; one had the desired medicinal properties whereas the other was later found to cause severe birth defects. Thus, the ability to manufacture drugs as single stereoisomers has become a critically important issue for the modern pharmaceutical industry.

It's more difficult to make a molecule as a single stereoisomer, however, Deslongchamps is developing computer-based tools and methods for doing just that – developing asymmetric organocatalysts (purely metal-free organic catalysts) that can produce a molecule of "single handedness". His is the only research group in the world retraining computer-based drug design tools for the purpose of organocatalyst discovery. Because organocatalysts are metal-free, they may produce less toxic and more environmentally sound drugs, important components of green chemistry.

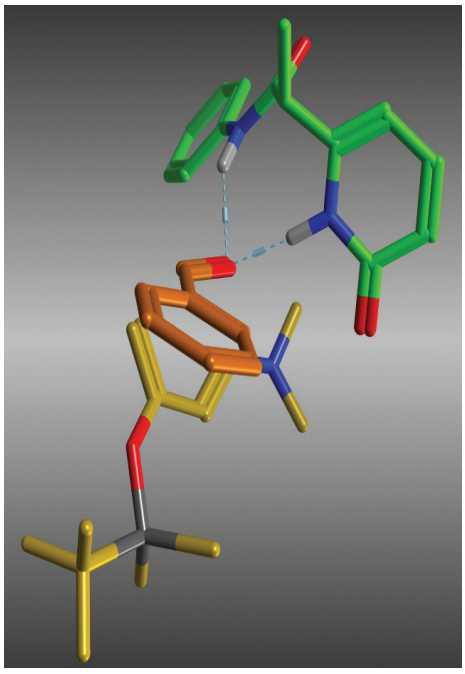
While the catalysts he is designing are of great interest to the pharmaceutical industry, his computational tools can also be applied to many other areas where molecules with very specific chemical shapes, features and properties are required.

The tools he's creating — one called "reverse-docking" and the other called "virtual screening" – are inspired by those used in computer-assisted drug design. The computations carried out in his lab can be extremely time onerous and require very advanced computing resources.

"We are extremely fortunate to be part of ACENET and having access to the Compute Canada resources to do the research that we do," Deslongchamps says. "A lot of the work we do might otherwise take months of calculating as opposed to days. It's almost impractical to do this research on a single computer."

Deslongchamps has a long-standing collaborative relationship with Chemical Computing Group Inc. (CCG), a leading drug software company based in Montreal. CCG is one of only a handful of such companies in the world and Dr. Deslongchamps is utilizing and adapting their software for designing and discovering new catalysts.

Dr. Deslongchamps has received additional computing resources for 2015 through Compute Canada's national Resource Allocation Competition.



Chiral organocatalyst (in green) catalyzing an asymmetric organic reaction. The organocatalyst was selected from a database containing millions of organic compounds using virtual screening and reverse-docking tools developed in the Deslongchamps group.

Pushing the Envelope (or Molecule) with Quantum Chemistry

Dr. Jason Pearson's research team of seven at the University of Prince Edward Island strives to understand the properties of molecules at the electronic level; why they behave the way they do, why some interactions are strong while others are not, and ultimately predict how molecules will behave when interacting with other molecules. It's a broad scope. They do this by developing and applying computational algorithms.

For example, an experimental researcher might have samples from which they are searching for new compounds. Along the way, they might find something with interesting properties, but need to identify the chemical substance. This is where Dr. Pearson's group can take the experimental data, build every possibility into models and then run simulations with the data that ultimately allows them to understand the molecule. Researchers then can examine the molecule through a new lens so to speak.

But it doesn't stop there. Along the way, Pearson is developing new computational tools and new simulation techniques useful for other researchers. Already a resource to colleagues at the University, Pearson's long-term focus is to utilize and develop computational technology for the purpose of designing new molecules and materials.

His group employs a two-pronged approach whereby state-of-the-art simulation techniques are applied to probe the molecular level of detail in chemical systems, allowing for accurate quantifications of structure, interactions, and mechanisms of action. Simultaneously, they design the next generation of computational algorithms and methodologies for the investigation of electronic structure, specifically focused on the concept of the electron pair.

The methods developed in his lab can be applied to almost all matter, and therefore can be used in many fields, such as designing new materials, new industrially relevant catalysts and nanotechnologies to name a few.

Pearson hopes to further push the bounds of what's possible in computational chemistry by gathering large datasets in the chemical sciences, creating a database for others to access and utilizing the data to develop new simulation techniques that are faster and more accurate. For example, this approach could enable very accurate simulations on large systems like biomolecules and other polymers. His goal is to develop algorithms that behave like a robot, travelling through the data sets, collecting data and solving problems.

The chemistry research that is enabled by Dr. Pearson's group is addressing a broad scope of the world's most important technological and societal challenges, such as climate change, energy, security, food supply and health.

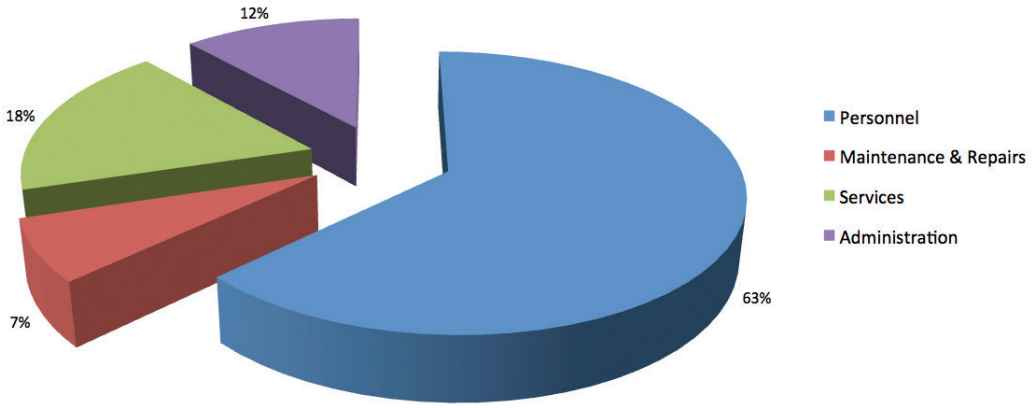
Financials

Financial Summary Report

April 1, 2014 - March 31, 2015

Expenses	Amounts	Notes
Personnel	$1,331,624	Includes staff at all five major resource provider Universities
Maintenance & Repairs	$152,275	Services Warranties, Replacement Parts
Services	$382,613	Software Licenses, Utilities, Telecommunications
Administration	$246,870	Supplies, Outreach, Marketing, Travel, HPCS 2014

Expenses 2014 - 2015



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